



Sample name: **M02_octanol** Experiment start time: **3/1/2018 2:44:22 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-01011** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

pH-metric Result

logP (XH +) 1.32 ±0.06 (n=50)
logP (neutral X) 4.10 ±0.03 (n=50)

18C-01011 Points 1 to 16

M02_octanol concentration factor 0.688
Carbonate 0.0278 mM
Acidity error -0.23518 mM

18C-01011 Points 17 to 26

M02_octanol concentration factor 0.751
Carbonate 0.1291 mM
Acidity error -0.36000 mM

18C-01011 Points 27 to 42

M02_octanol concentration factor 0.599
Carbonate 0.0511 mM
Acidity error -0.26646 mM

Warnings and errors

Errors None
Warnings None

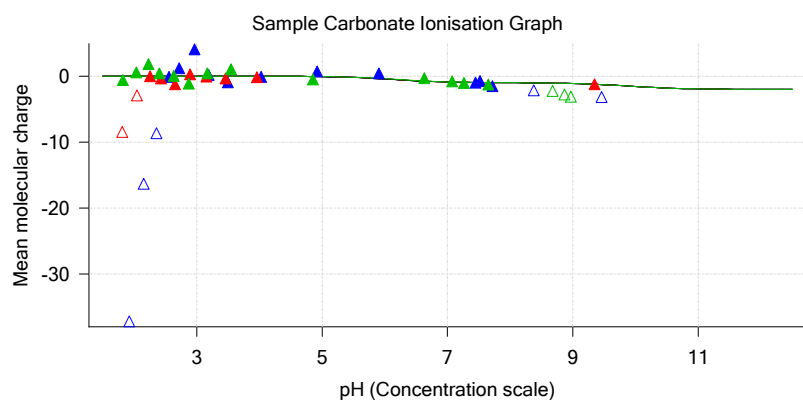
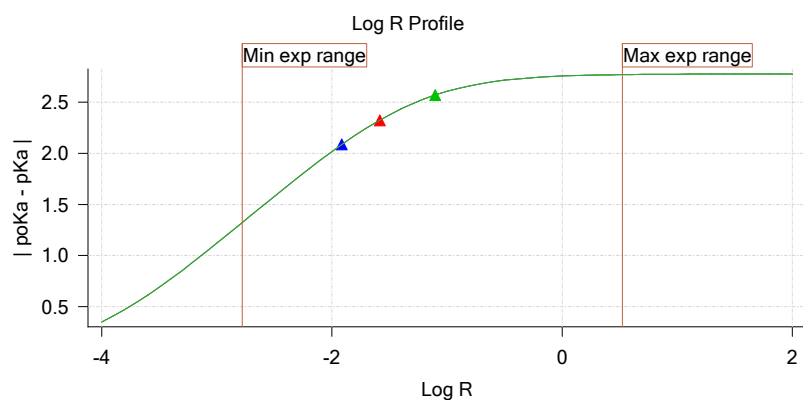
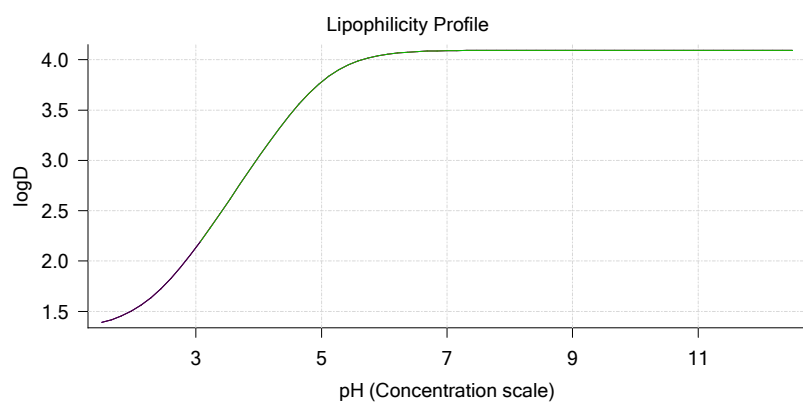
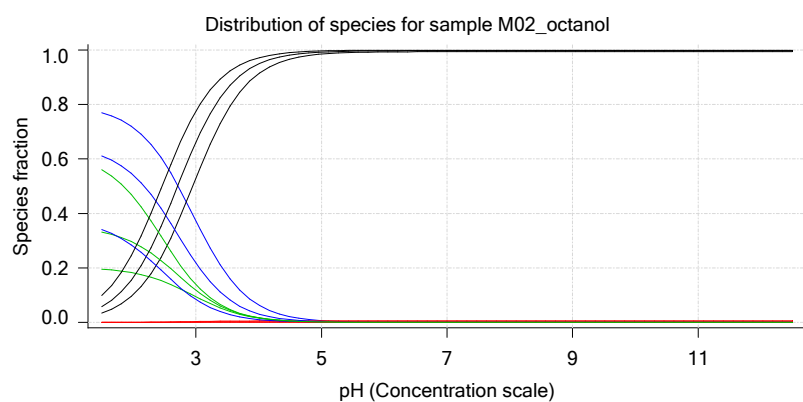
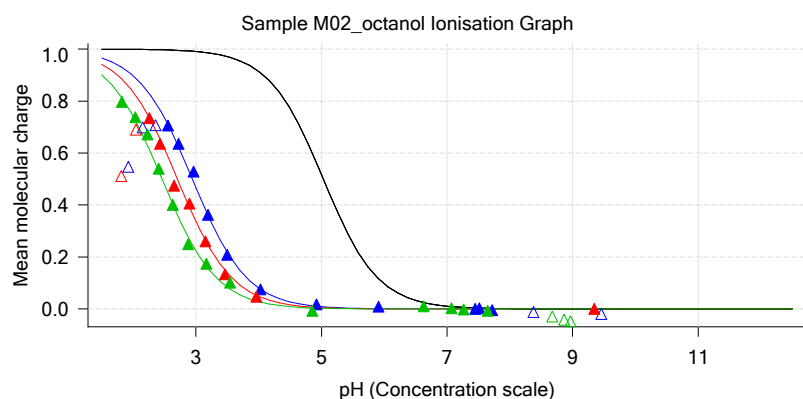
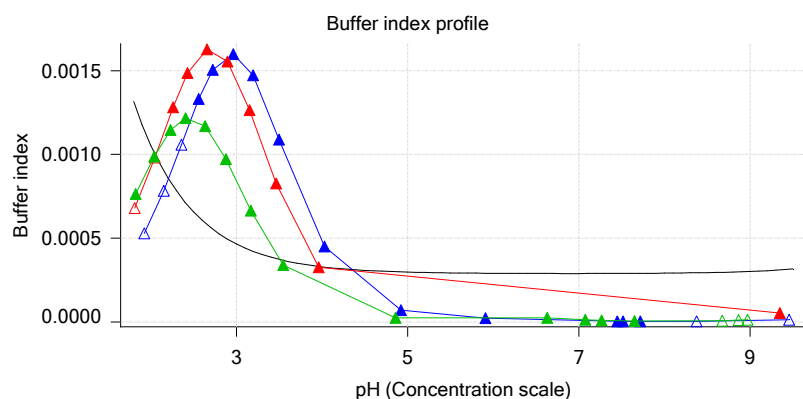
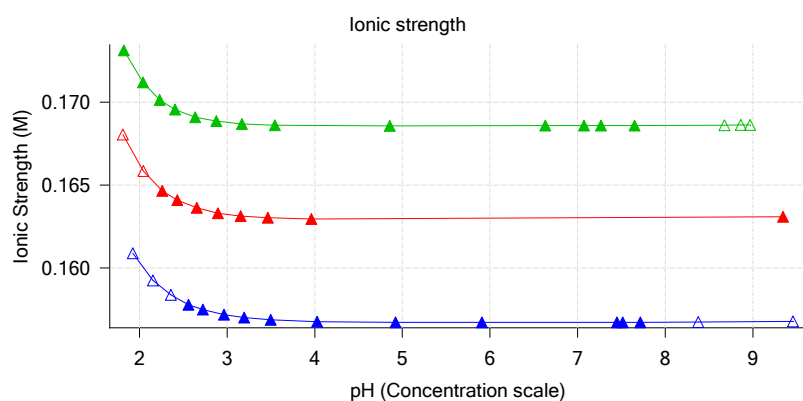
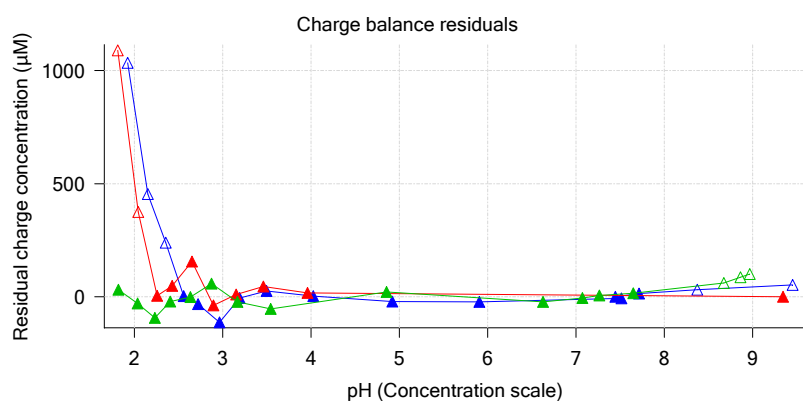
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.34	4.34 %	0.00 %	90.61 %	5.05 %	Stomach pH
1.200	1.36	4.22 %	0.00 %	88.01 %	7.77 %	
2.000	1.51	2.99 %	0.00 %	62.31 %	34.70 %	
3.000	2.13	0.72 %	0.01 %	15.11 %	84.16 %	
4.000	3.03	0.08 %	0.01 %	1.76 %	98.15 %	
5.000	3.78	0.01 %	0.01 %	0.18 %	99.80 %	Blood pH
6.000	4.05	0.00 %	0.01 %	0.02 %	99.97 %	
6.500	4.08	0.00 %	0.01 %	0.01 %	99.99 %	
7.000	4.09	0.00 %	0.01 %	0.00 %	99.99 %	
7.400	4.09	0.00 %	0.01 %	0.00 %	99.99 %	
8.000	4.09	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	4.10	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	4.10	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	4.10	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	4.10	0.00 %	0.01 %	0.00 %	99.99 %	

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

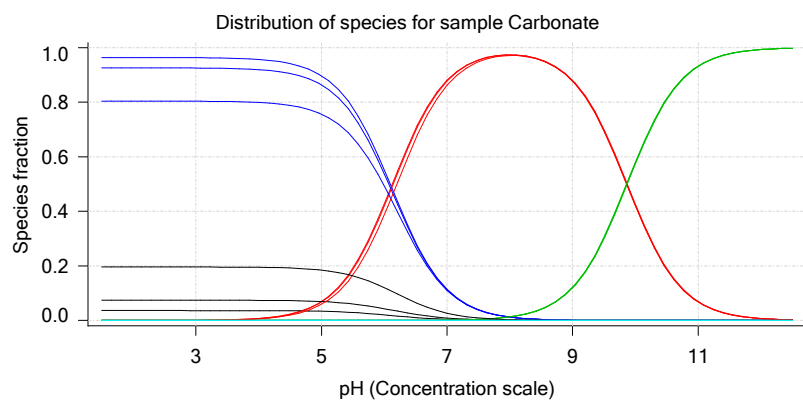
Graphs



Sample name: **M02_octanol**
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 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
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 Instrument ID: **T312060**

Graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-01011 Points 1 to 16

Overall results

RMSD 1.164
 Average ionic strength 0.157 M
 Average temperature 24.9°C
 Partition ratio 0.0122 : 1
 Analyte concentration range 3971.1 µM to 4077.5 µM
 Total points considered 11 of 16

Warnings and errors

Errors None
 Warnings Sample concentration factor out of range

Four-Plus parameters

Alpha 0.130 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r

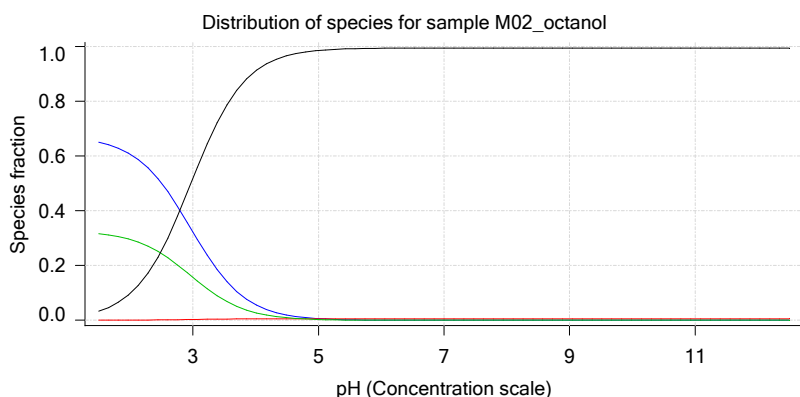
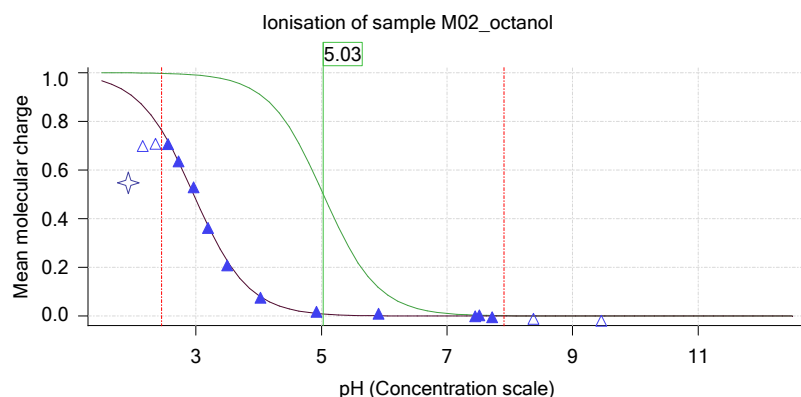
Titrants

0.50 M HCl 0.993513 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 3/1/2018 2:44:22 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M02_octanol concentration factor 0.688
 Base pKa 1 5.03
 logP (XH +) 1.60
 logP (neutral X) 4.15

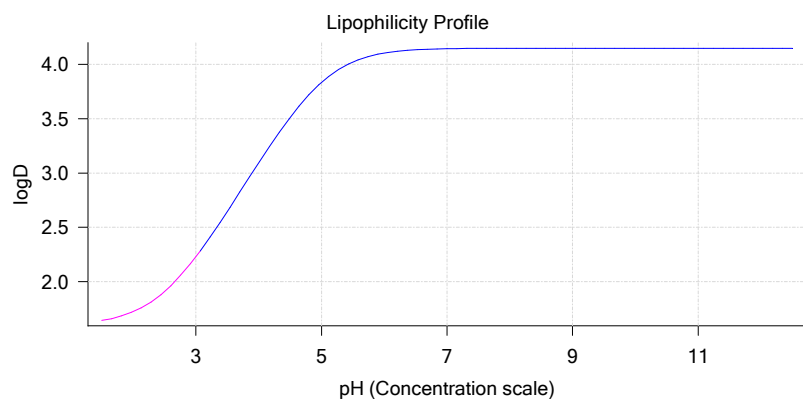
Sample graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**


Sample graphs (continued)



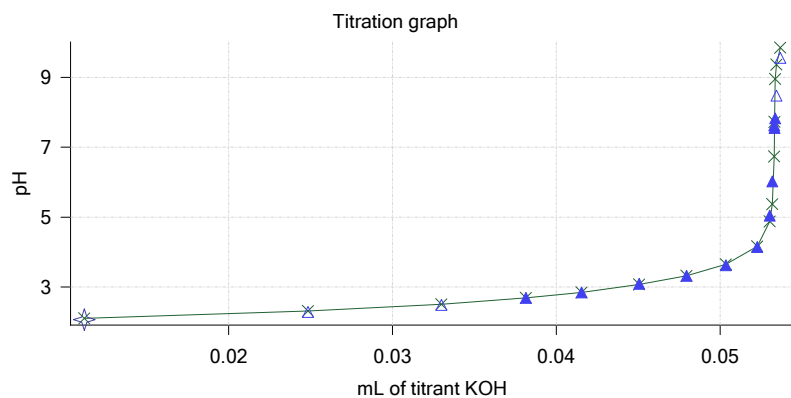
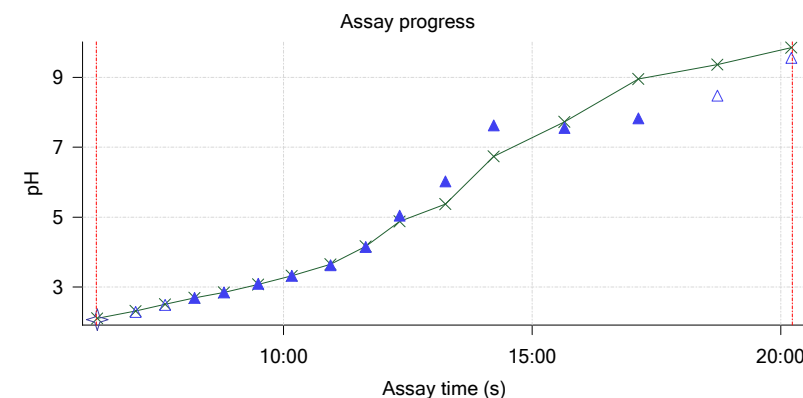
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.61	66.58 %	0.01 %	32.35 %	1.07 %	Stomach pH
1.200	1.62	66.16 %	0.01 %	32.15 %	1.68 %	
2.000	1.72	60.71 %	0.06 %	29.50 %	9.74 %	
3.000	2.23	32.27 %	0.30 %	15.68 %	51.75 %	
4.000	3.09	5.68 %	0.53 %	2.76 %	91.04 %	
5.000	3.83	0.61 %	0.57 %	0.30 %	98.51 %	Blood pH
6.000	4.10	0.06 %	0.58 %	0.03 %	99.33 %	
6.500	4.13	0.02 %	0.58 %	0.01 %	99.39 %	
7.000	4.14	0.01 %	0.58 %	0.00 %	99.41 %	
7.400	4.15	0.00 %	0.58 %	0.00 %	99.42 %	
8.000	4.15	0.00 %	0.58 %	0.00 %	99.42 %	
9.000	4.15	0.00 %	0.58 %	0.00 %	99.42 %	
10.000	4.15	0.00 %	0.58 %	0.00 %	99.42 %	
11.000	4.15	0.00 %	0.58 %	0.00 %	99.42 %	
12.000	4.15	0.00 %	0.58 %	0.00 %	99.42 %	

Carbonate and acidity

 Carbonate 0.028 mM
 Acidity error -0.235 mM

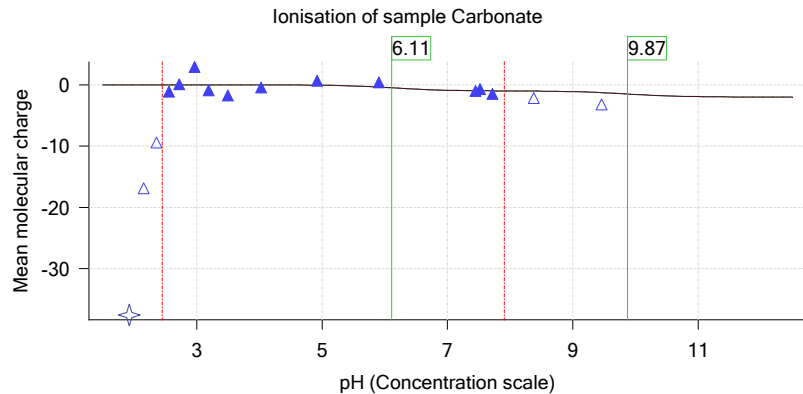
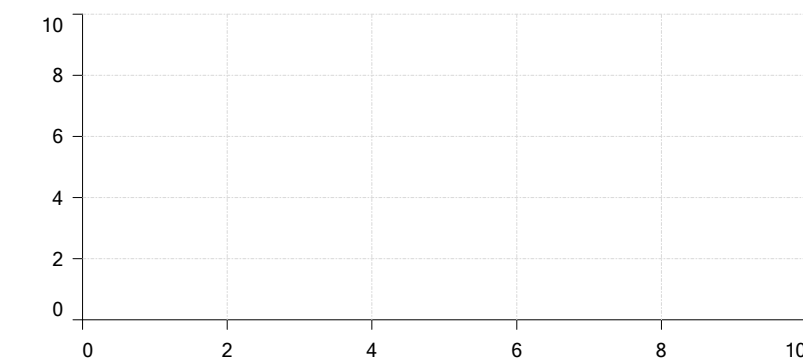
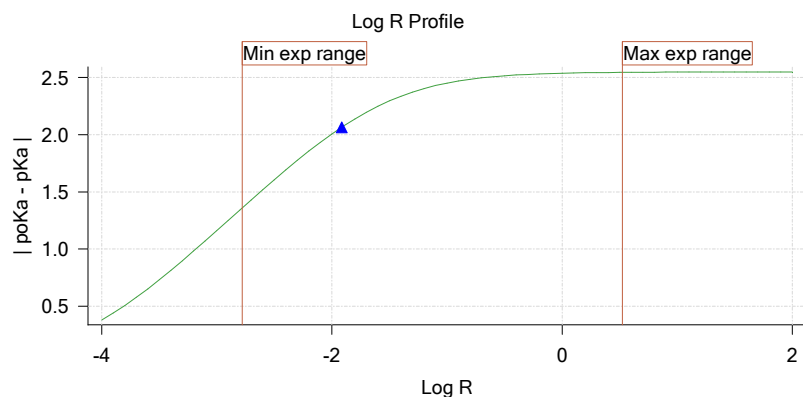
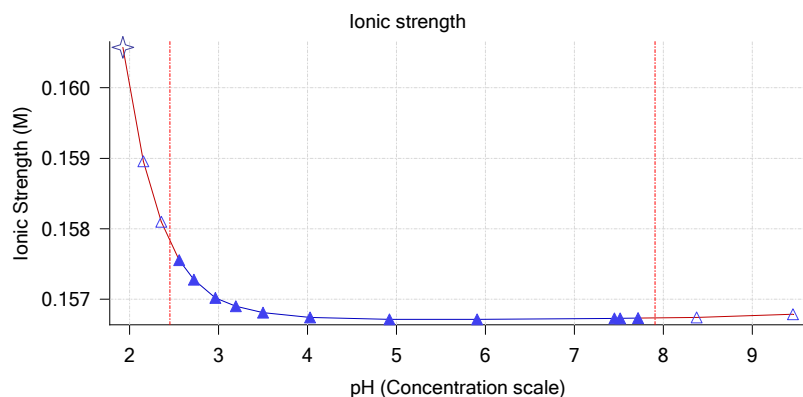
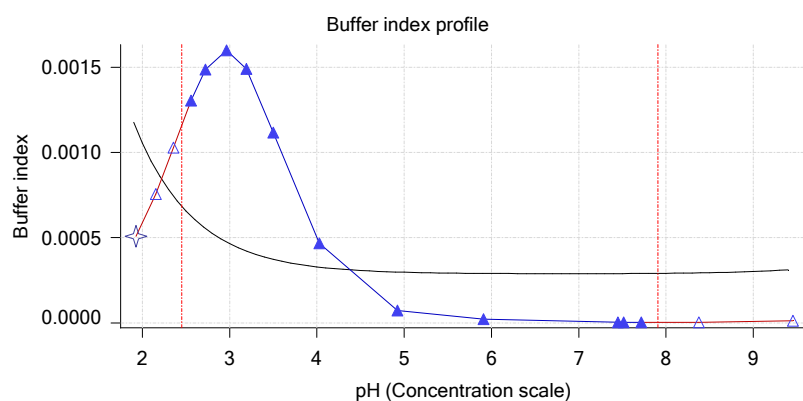
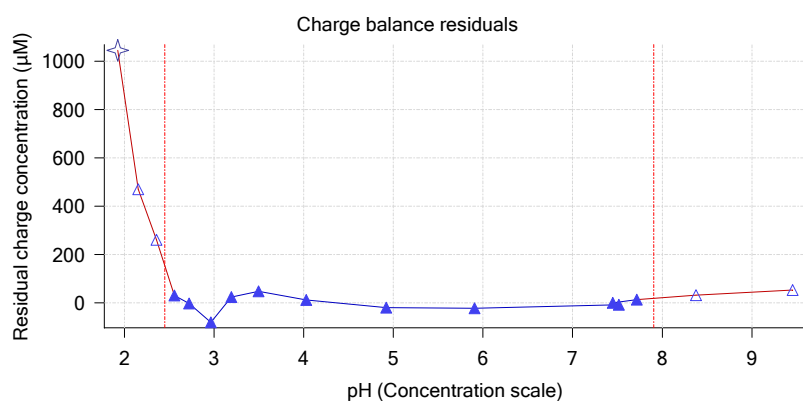
Other graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
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 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-01011 Points 17 to 26

Overall results

RMSD 0.012
 Average ionic strength 0.163 M
 Average temperature 25.0°C
 Partition ratio 0.0260 : 1
 Analyte concentration range 3657.5 µM to 3779.3 µM
 Total points considered 8 of 10

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.130 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r

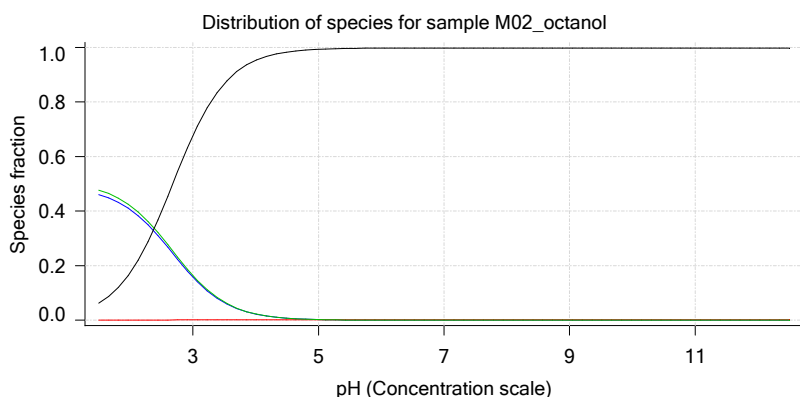
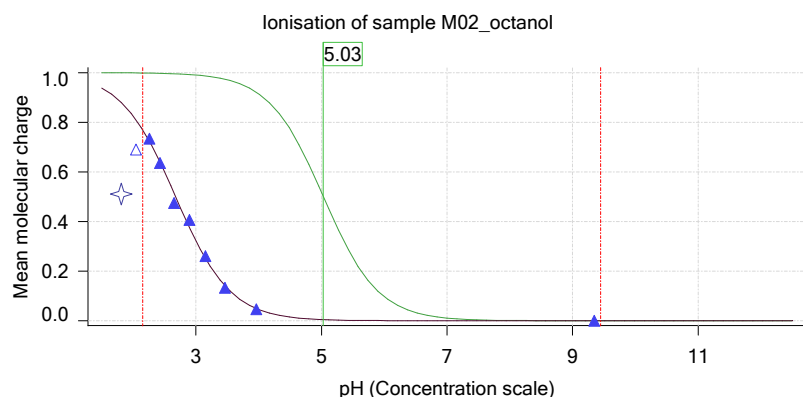
Titrants

0.50 M HCl 0.993513 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 3/1/2018 2:44:22 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M02_octanol concentration factor 0.751
 Base pKa 1 5.03
 logP (XH +) 1.60
 logP (neutral X) 4.25

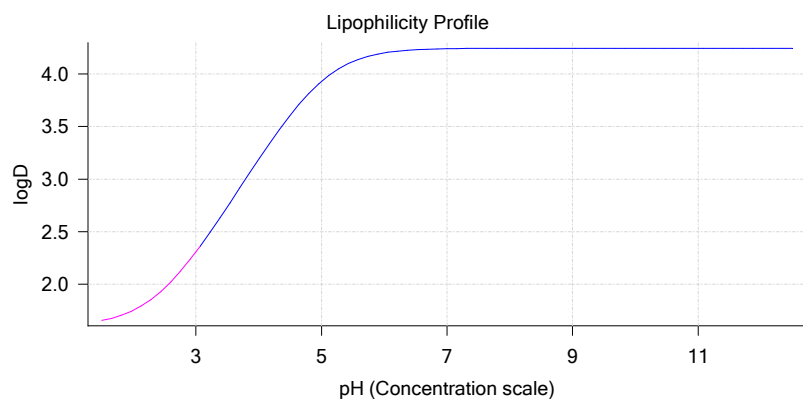
Sample graphs



Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Sample graphs (continued)



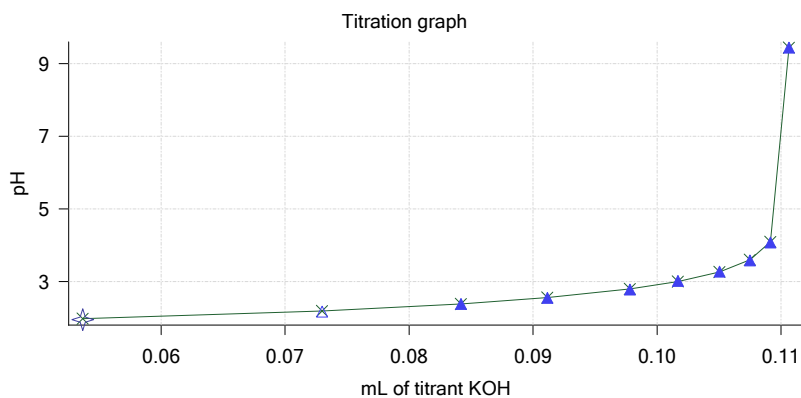
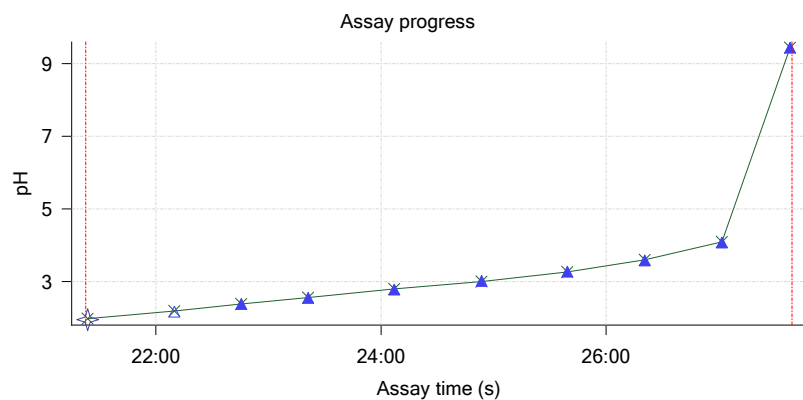
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.62	48.12 %	0.00 %	49.81 %	2.06 %	
1.200	1.63	47.55 %	0.01 %	49.22 %	3.23 %	
2.000	1.75	40.58 %	0.04 %	42.01 %	17.38 %	
3.000	2.31	15.81 %	0.15 %	16.36 %	67.68 %	
4.000	3.19	2.22 %	0.21 %	2.30 %	95.26 %	
5.000	3.93	0.23 %	0.22 %	0.24 %	99.31 %	
6.000	4.20	0.02 %	0.22 %	0.02 %	99.74 %	
6.500	4.23	0.01 %	0.22 %	0.01 %	99.77 %	
7.000	4.24	0.00 %	0.22 %	0.00 %	99.78 %	
7.400	4.24	0.00 %	0.22 %	0.00 %	99.78 %	
8.000	4.25	0.00 %	0.22 %	0.00 %	99.78 %	
9.000	4.25	0.00 %	0.22 %	0.00 %	99.78 %	
10.000	4.25	0.00 %	0.22 %	0.00 %	99.78 %	
11.000	4.25	0.00 %	0.22 %	0.00 %	99.78 %	
12.000	4.25	0.00 %	0.22 %	0.00 %	99.78 %	

Carbonate and acidity

Carbonate 0.129 mM
Acidity error -0.360 mM

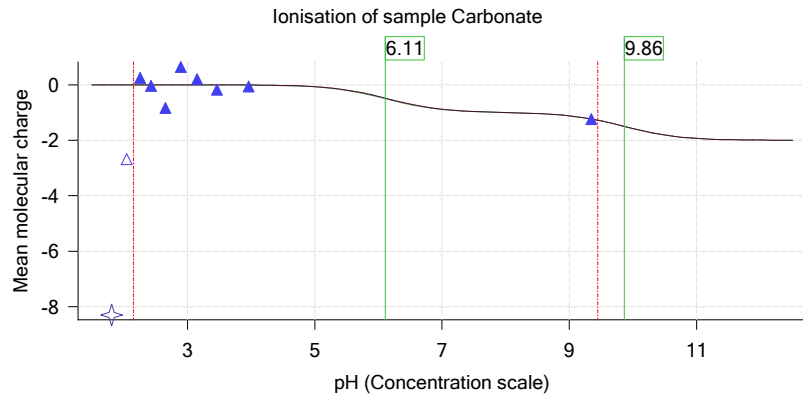
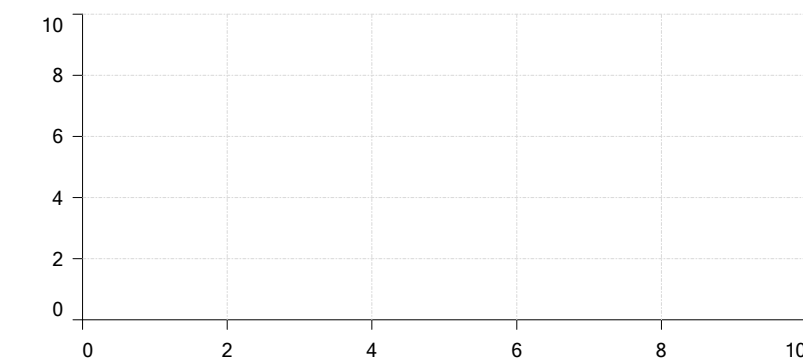
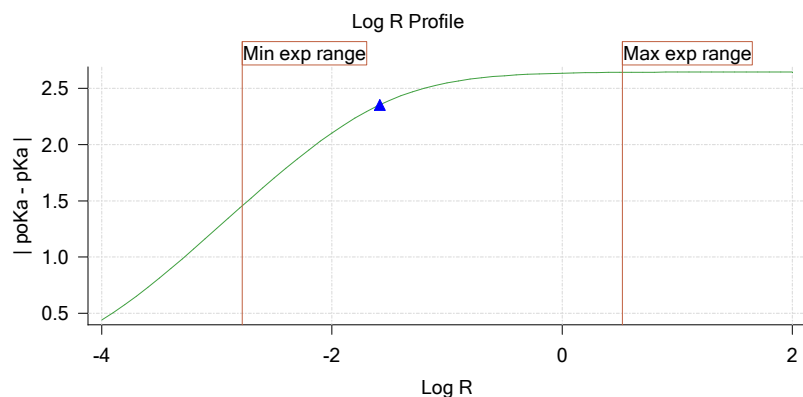
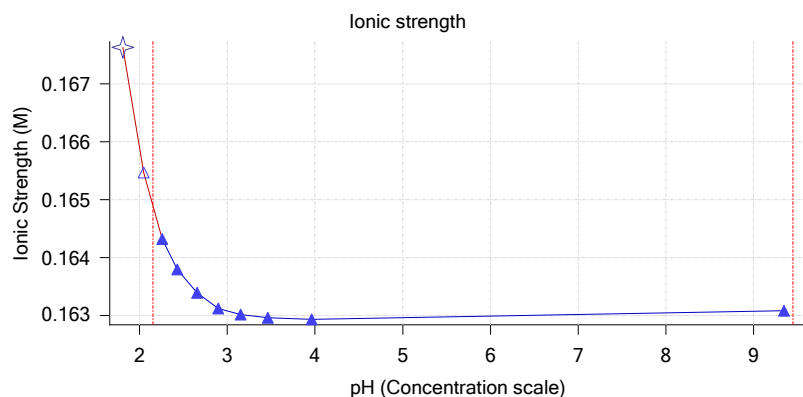
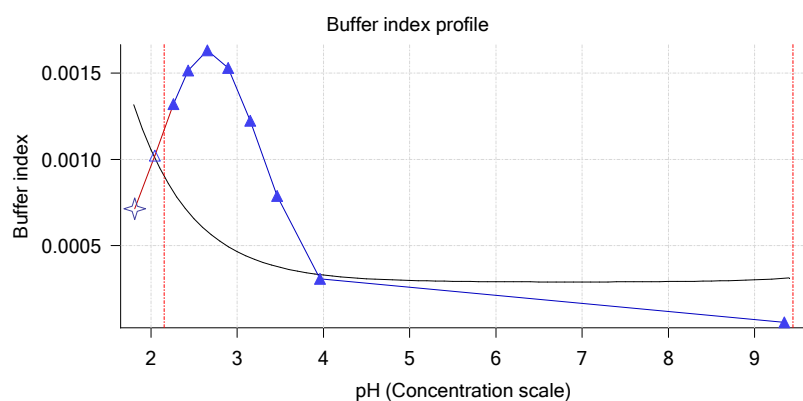
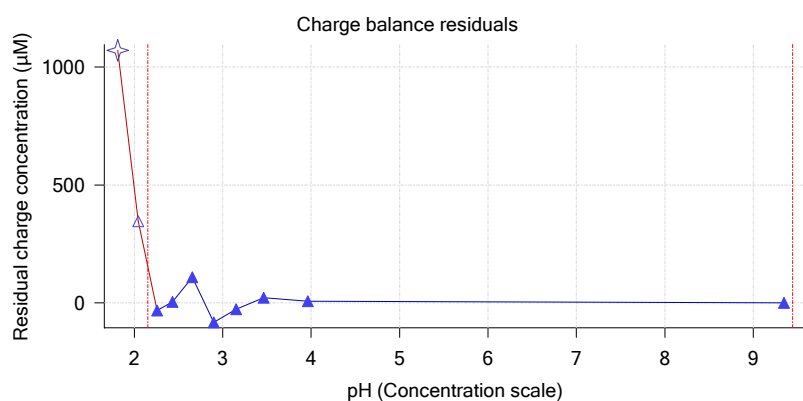
Other graphs



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 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

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Other graphs (continued)



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 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-01011 Points 27 to 42

Overall results

RMSD 0.734
 Average ionic strength 0.169 M
 Average temperature 25.0°C
 Partition ratio 0.0789 : 1
 Analyte concentration range 3250.6 µM to 3352.6 µM
 Total points considered 13 of 16

Warnings and errors

Errors None
 Warnings Sample concentration factor out of range

Four-Plus parameters

Alpha 0.130 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r

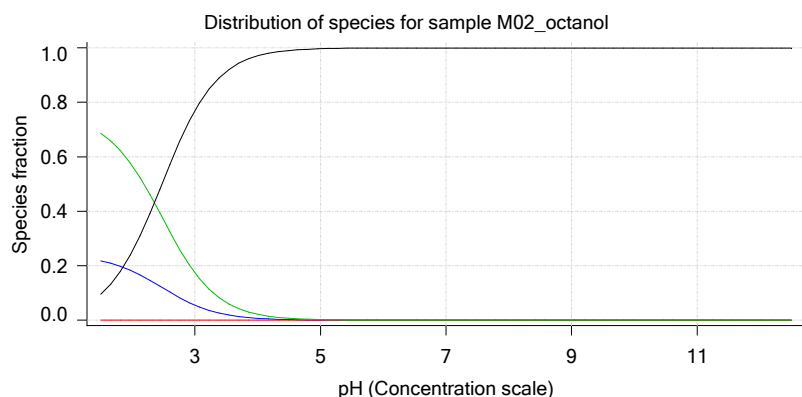
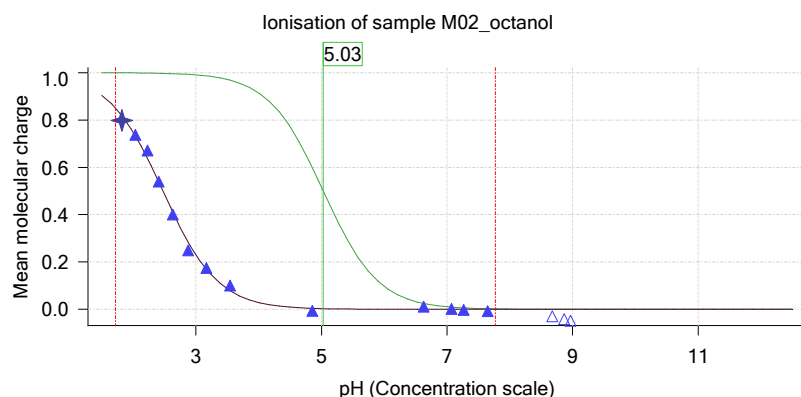
Titrants

0.50 M HCl 0.993513 3/1/2018 2:44:22 PM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 3/1/2018 2:44:22 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M02_octanol concentration factor 0.599
 Base pKa 1 5.03
 logP (XH +) 1.60
 logP (neutral X) 4.27

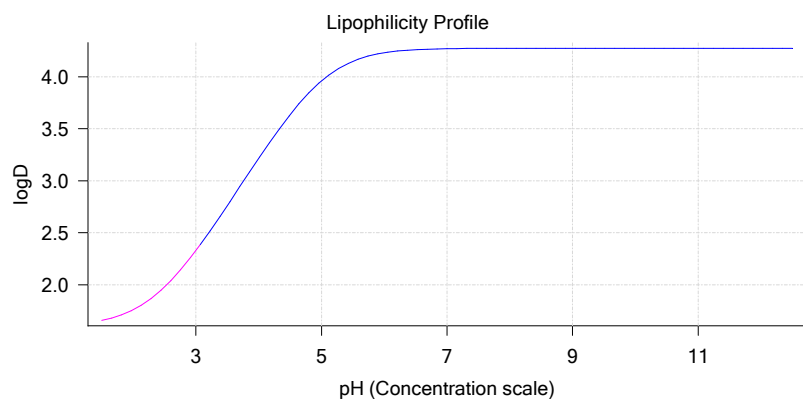
Sample graphs



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 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
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Sample graphs (continued)



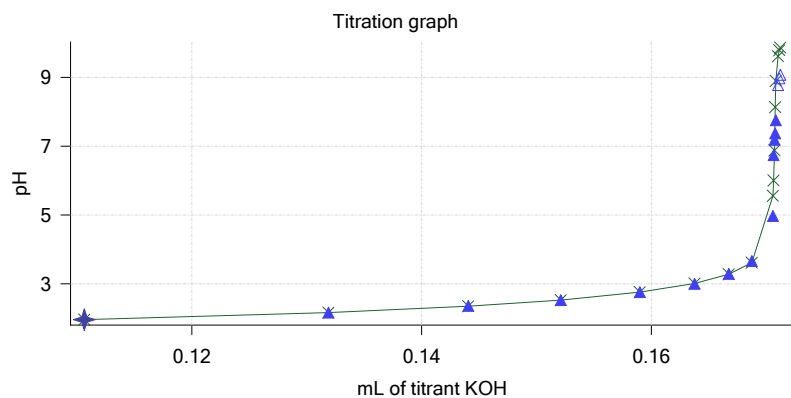
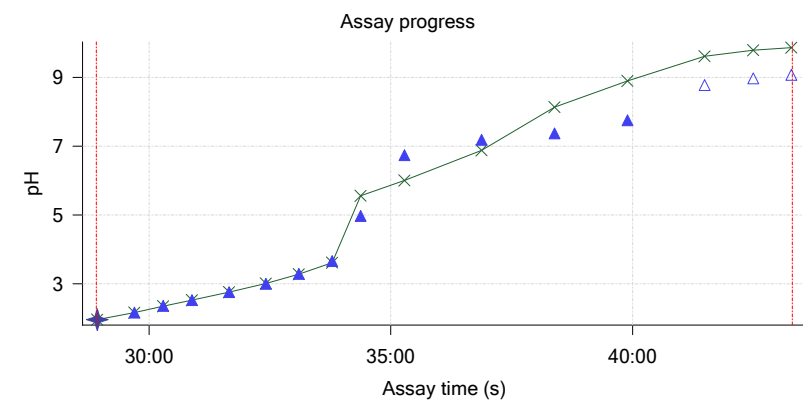
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.62	23.36 %	0.00 %	73.40 %	3.24 %	Stomach pH
1.200	1.63	22.92 %	0.00 %	72.04 %	5.04 %	
2.000	1.76	18.08 %	0.02 %	56.83 %	25.06 %	
3.000	2.33	5.55 %	0.05 %	17.45 %	76.95 %	
4.000	3.22	0.70 %	0.07 %	2.20 %	97.03 %	
5.000	3.96	0.07 %	0.07 %	0.23 %	99.64 %	Blood pH
6.000	4.23	0.01 %	0.07 %	0.02 %	99.90 %	
6.500	4.26	0.00 %	0.07 %	0.01 %	99.92 %	
7.000	4.27	0.00 %	0.07 %	0.00 %	99.93 %	
7.400	4.27	0.00 %	0.07 %	0.00 %	99.93 %	
8.000	4.27	0.00 %	0.07 %	0.00 %	99.93 %	
9.000	4.27	0.00 %	0.07 %	0.00 %	99.93 %	
10.000	4.27	0.00 %	0.07 %	0.00 %	99.93 %	
11.000	4.27	0.00 %	0.07 %	0.00 %	99.93 %	
12.000	4.27	0.00 %	0.07 %	0.00 %	99.93 %	

Carbonate and acidity

 Carbonate 0.051 mM
 Acidity error -0.266 mM

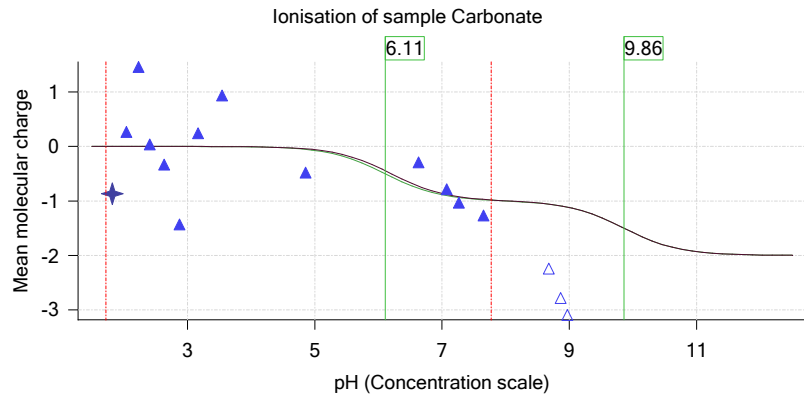
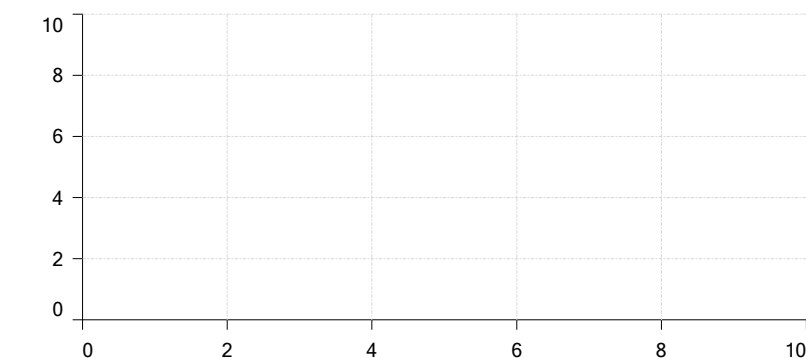
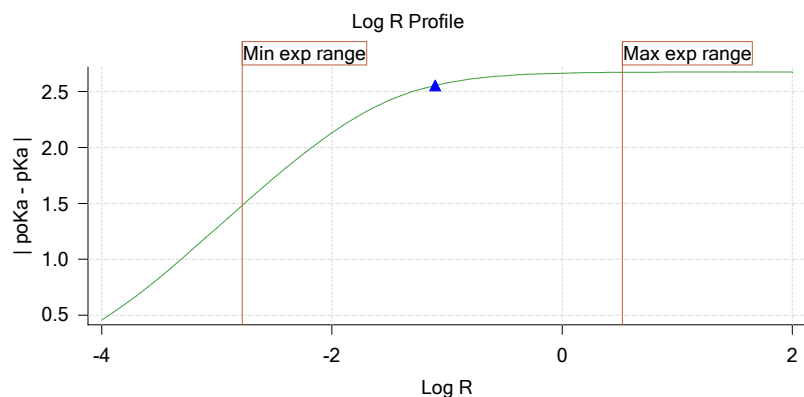
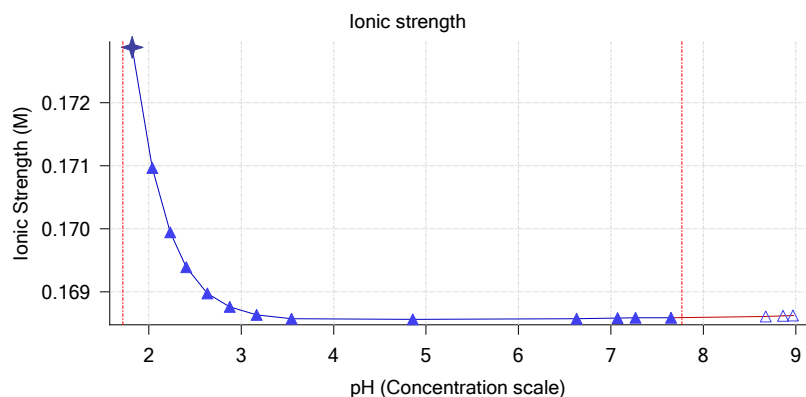
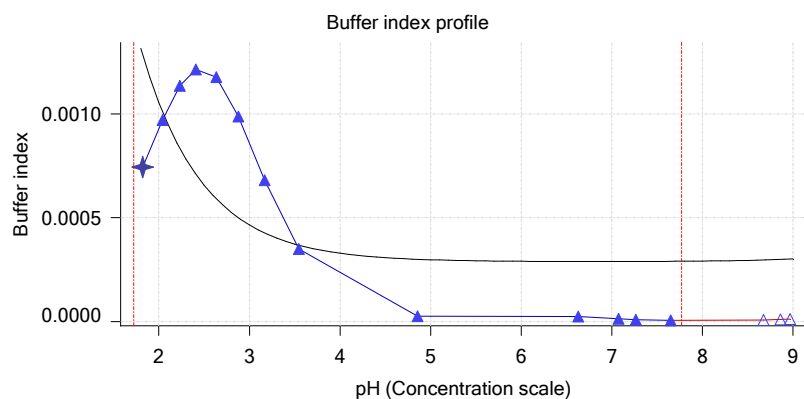
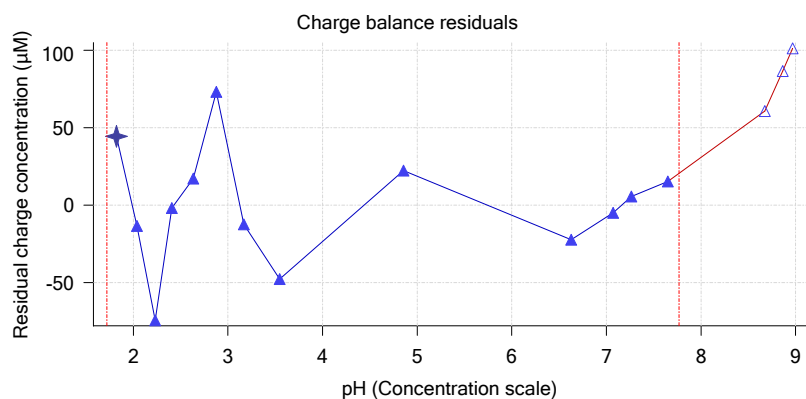
Other graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T312060**

Other graphs (continued)





Sample name: **M02_octanol** Experiment start time: **3/1/2018 2:44:22 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-01011** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M02_octanol	12/6/2017 4:20:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001870 g	2/28/2018 4:51:34 PM	User entered value
Formula weight	289.26 g/mol	12/6/2017 4:20:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	289.26	12/6/2017 4:20:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	12/6/2017 4:20:03 PM	User entered value
Sample is a	Base	12/6/2017 4:20:03 PM	User entered value
pKa 1	5.03	12/6/2017 4:20:03 PM	User entered value
logp (XH +)	1.60	12/6/2017 4:20:17 PM	User entered value
logP (neutral X)	3.00	2/28/2018 2:50:25 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
3:15.5	Initial pH = 6.92									
6:15.3	Data point 1	1.50000 mL	0.05433 mL	0.01119 mL	0.01999 mL	2.059	0.00260	0.18062	0.00030	10.0 s
7:01.6	Data point 2	1.50000 mL	0.05433 mL	0.02484 mL	0.01999 mL	2.282	0.00555	0.77597	0.00031	10.0 s
7:37.2	Data point 3	1.50000 mL	0.05433 mL	0.03300 mL	0.01999 mL	2.484	0.01434	0.77758	0.00080	10.0 s
8:12.8	Data point 4	1.50000 mL	0.05433 mL	0.03815 mL	0.01999 mL	2.683	0.00592	0.63815	0.00037	10.0 s
8:48.3	Data point 5	1.50000 mL	0.05433 mL	0.04153 mL	0.01999 mL	2.846	-0.00121	0.24285	0.00012	10.5 s
9:29.5	Data point 6	1.50000 mL	0.05433 mL	0.04506 mL	0.01999 mL	3.087	-0.00967	0.98095	0.00048	10.0 s
10:10.2	Data point 7	1.50000 mL	0.05433 mL	0.04795 mL	0.01999 mL	3.314	-0.01605	0.70172	0.00095	16.0 s
10:56.9	Data point 8	1.50000 mL	0.05433 mL	0.05035 mL	0.01999 mL	3.619	-0.01833	0.92570	0.00094	11.5 s
11:39.2	Data point 9	1.50000 mL	0.05433 mL	0.05226 mL	0.01999 mL	4.146	-0.01442	0.66678	0.00087	15.5 s
12:20.1	Data point 10	1.50000 mL	0.05433 mL	0.05303 mL	0.01999 mL	5.037	-0.01988	0.98479	0.00099	25.0 s
13:15.6	Data point 11	1.50000 mL	0.05433 mL	0.05318 mL	0.01999 mL	6.020	-0.01461	0.67162	0.00088	27.5 s
14:13.7	Data point 12	1.50000 mL	0.05433 mL	0.05329 mL	0.01999 mL	7.623	-0.08314	0.99820	0.00411	Timed out at 59.5 s
15:39.0	Data point 13	1.50000 mL	0.05433 mL	0.05332 mL	0.01999 mL	7.556	-0.01960	0.99189	0.00097	58.5 s
17:08.1	Data point 14	1.50000 mL	0.05433 mL	0.05336 mL	0.01999 mL	7.824	-0.04269	0.97447	0.00214	Timed out at 59.5 s
18:43.7	Data point 15	1.50000 mL	0.05433 mL	0.05343 mL	0.01999 mL	8.480	-0.01896	0.89770	0.00099	53.5 s
20:12.9	Data point 16	1.50000 mL	0.05433 mL	0.05367 mL	0.01999 mL	9.557	-0.01673	0.69489	0.00099	17.0 s
21:23.5	Data point 17	1.50000 mL	0.11192 mL	0.05367 mL	0.04499 mL	1.948	0.00696	0.77037	0.00039	10.0 s
22:09.8	Data point 18	1.50000 mL	0.11192 mL	0.07298 mL	0.04499 mL	2.177	0.01234	0.90932	0.00064	10.0 s
22:45.5	Data point 19	1.50000 mL	0.11192 mL	0.08420 mL	0.04499 mL	2.387	-0.00583	0.35938	0.00048	10.0 s
23:21.1	Data point 20	1.50000 mL	0.11192 mL	0.09116 mL	0.04499 mL	2.556	0.00696	0.30662	0.00062	10.0 s
24:07.1	Data point 21	1.50000 mL	0.11192 mL	0.09781 mL	0.04499 mL	2.779	0.00229	0.34291	0.00019	10.5 s
24:53.5	Data point 22	1.50000 mL	0.11192 mL	0.10169 mL	0.04499 mL	3.019	-0.00417	0.40847	0.00032	10.0 s
25:39.4	Data point 23	1.50000 mL	0.11192 mL	0.10503 mL	0.04499 mL	3.274	-0.00304	0.48058	0.00022	10.5 s
26:20.5	Data point 24	1.50000 mL	0.11192 mL	0.10750 mL	0.04499 mL	3.583	-0.01595	0.64072	0.00098	10.5 s
27:01.7	Data point 25	1.50000 mL	0.11192 mL	0.10915 mL	0.04499 mL	4.080	-0.00893	0.27765	0.00084	11.0 s
27:38.1	Data point 26	1.50000 mL	0.11192 mL	0.11065 mL	0.04499 mL	9.447	-0.01272	0.80417	0.00070	22.0 s
28:55.6	Data point 27	1.50000 mL	0.17265 mL	0.11065 mL	0.14499 mL	1.958	-0.00711	0.87945	0.00037	10.0 s
29:41.9	Data point 28	1.50000 mL	0.17265 mL	0.13189 mL	0.14499 mL	2.170	0.00288	0.03386	0.00077	10.0 s
30:17.6	Data point 29	1.50000 mL	0.17265 mL	0.14407 mL	0.14499 mL	2.360	0.00992	0.49242	0.00070	10.0 s
30:53.2	Data point 30	1.50000 mL	0.17265 mL	0.15212 mL	0.14499 mL	2.533	-0.00071	0.03478	0.00019	10.0 s
31:39.2	Data point 31	1.50000 mL	0.17265 mL	0.15898 mL	0.14499 mL	2.759	-0.00280	0.03542	0.00073	10.0 s
32:25.2	Data point 32	1.50000 mL	0.17265 mL	0.16376 mL	0.14499 mL	2.999	0.00572	0.11987	0.00082	10.0 s
33:05.9	Data point 33	1.50000 mL	0.17265 mL	0.16672 mL	0.14499 mL	3.289	-0.00045	0.04094	0.00011	10.5 s
33:47.1	Data point 34	1.50000 mL	0.17265 mL	0.16874 mL	0.14499 mL	3.666	-0.00646	0.91671	0.00033	10.0 s
34:22.5	Data point 35	1.50000 mL	0.17265 mL	0.17058 mL	0.14499 mL	4.972	-0.01889	0.93768	0.00096	29.0 s
35:16.9	Data point 36	1.50000 mL	0.17265 mL	0.17063 mL	0.14499 mL	6.740	-0.05158	0.98694	0.00256	Timed out at 59.5 s
36:52.5	Data point 37	1.50000 mL	0.17265 mL	0.17072 mL	0.14499 mL	7.181	-0.03986	0.97488	0.00199	Timed out at 59.5 s



Assay Events

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
38:23.1	Data point 38	1.50000 mL	0.17265 mL	0.17077 mL	0.14499 mL	7.373	-0.03900	0.95207	0.00197	Timed out at 59.5 s
39:53.6	Data point 39	1.50000 mL	0.17265 mL	0.17081 mL	0.14499 mL	7.756	-0.05606	0.98714	0.00279	Timed out at 59.5 s
41:29.3	Data point 40	1.50000 mL	0.17265 mL	0.17103 mL	0.14499 mL	8.778	-0.01761	0.76339	0.00100	24.5 s
42:29.5	Data point 41	1.50000 mL	0.17265 mL	0.17114 mL	0.14499 mL	8.966	-0.01729	0.75749	0.00098	17.0 s
43:17.1	Data point 42	1.50000 mL	0.17265 mL	0.17121 mL	0.14499 mL	9.071	-0.01579	0.68970	0.00094	23.0 s
43:49.1	Assay volumes	1.50000 mL	0.17265 mL	0.17121 mL	0.14499 mL					

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	10%			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.025 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			
Titration 3				

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	3/1/2018 2:44:22 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 2:44:22 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 2:44:22 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 2:44:22 PM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 2:44:22 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 2:44:22 PM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM
Syringe volume	0.5 mL		

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titration		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+3.14 mV		3/1/2018 2:44:50 PM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Triton X-100 in H2O		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.1e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	7.3e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		

Sample name: **M02_octanol** Experiment start time: **3/1/2018 2:44:22 PM**
 Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
 Assay ID: **18C-01011** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
 [2:38] Air gap created for Acid (0.5 M HCl)
 [2:38] Air gap created for Base (0.5 M KOH)
 [2:38] Air gap released for Water (0.15 M KCl)
 [2:43] Titrator arm moved to Titration position
 [2:43] Argon flow rate set to 100
 [2:43] Titration 1 of 3
 [2:43] Adding initial titrants
 [2:43] Automatically add 1.50000 mL of water
 [3:09] Dispensed 1.500000 mL of Water (0.15 M KCl)
 [3:09] Stirrer speed set to 10
 [3:14] Automatically add 0.02000 mL of Octanol
 [3:14] Dispensed 0.019991 mL of Octanol
 [3:15] Initial pH = 6.92
 [3:15] Iterative adjust 6.92 -> 2.00
 [3:15] pH 6.92 -> 2.00
 [3:17] Air gap released for Acid (0.5 M HCl)
 [3:18] Dispensed 0.054327 mL of Acid (0.5 M HCl)
 [3:23] Holding pH 2.00
 [5:23] Stirrer speed set to 0
 [5:23] Stirrer speed set to 50
 [5:23] Iterative adjust 1.90 -> 2.00
 [5:23] pH 1.90 -> 2.00
 [5:24] Air gap released for Base (0.5 M KOH)
 [5:25] Dispensed 0.011195 mL of Base (0.5 M KOH)
 [6:15] Stirrer speed set to 0
 [6:25] Datapoint id 1 collected
 [6:25] Stirrer speed set to 50
 [6:30] pH 2.07 -> 2.27
 [6:30] Using cautious pH adjust
 [6:31] Dispensed 0.006867 mL of Base (0.5 M KOH)
 [6:36] Stepping pH = 2.15
 [6:36] Dispensed 0.005386 mL of Base (0.5 M KOH)
 [6:41] Stepping pH = 2.24
 [6:41] Dispensed 0.001388 mL of Base (0.5 M KOH)
 [6:46] Stepping pH = 2.27
 [7:02] Stirrer speed set to 0
 [7:12] Datapoint id 2 collected
 [7:12] Charge balance equation is out by 0.6%
 [7:12] Stirrer speed set to 50
 [7:17] pH 2.29 -> 2.49
 [7:17] Using charge balance adjust
 [7:17] Dispensed 0.008161 mL of Base (0.5 M KOH)

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[7:37] Stirrer speed set to 0
[7:47] Datapoint id 3 collected
[7:47] Charge balance equation is out by -4.6%
[7:47] Stirrer speed set to 50
[7:52] pH 2.50 -> 2.70
[7:52] Using charge balance adjust
[7:53] Dispensed 0.005151 mL of Base (0.5 M KOH)
[8:13] Stirrer speed set to 0
[8:23] Datapoint id 4 collected
[8:23] Charge balance equation is out by -7.3%
[8:23] Stirrer speed set to 50
[8:28] pH 2.70 -> 2.90
[8:28] Using charge balance adjust
[8:28] Dispensed 0.003387 mL of Base (0.5 M KOH)
[8:48] Stirrer speed set to 0
[8:59] Datapoint id 5 collected
[8:59] Charge balance equation is out by -24.9%
[8:59] Stirrer speed set to 50
[9:04] pH 2.86 -> 3.06
[9:04] Using cautious pH adjust
[9:04] Dispensed 0.001246 mL of Base (0.5 M KOH)
[9:09] Stepping pH = 2.89
[9:09] Dispensed 0.002281 mL of Base (0.5 M KOH)
[9:14] Stepping pH = 3.07
[9:29] Stirrer speed set to 0
[9:39] Datapoint id 6 collected
[9:39] Charge balance equation is out by -41.5%
[9:39] Stirrer speed set to 50
[9:45] pH 3.10 -> 3.30
[9:45] Using cautious pH adjust
[9:45] Dispensed 0.000870 mL of Base (0.5 M KOH)
[9:50] Stepping pH = 3.12
[9:50] Dispensed 0.002023 mL of Base (0.5 M KOH)
[9:55] Stepping pH = 3.29
[10:10] Stirrer speed set to 0
[10:26] Datapoint id 7 collected
[10:26] Charge balance equation is out by -66.6%
[10:26] Stirrer speed set to 50
[10:31] pH 3.33 -> 3.53
[10:31] Using cautious pH adjust
[10:31] Dispensed 0.000729 mL of Base (0.5 M KOH)
[10:36] Stepping pH = 3.36
[10:37] Dispensed 0.001670 mL of Base (0.5 M KOH)
[10:42] Stepping pH = 3.58
[10:57] Stirrer speed set to 0
[11:08] Datapoint id 8 collected
[11:08] Charge balance equation is out by -63.8%
[11:08] Stirrer speed set to 50
[11:13] pH 3.65 -> 3.85
[11:13] Using cautious pH adjust
[11:14] Dispensed 0.000753 mL of Base (0.5 M KOH)
[11:19] Stepping pH = 3.70
[11:19] Dispensed 0.001152 mL of Base (0.5 M KOH)
[11:24] Stepping pH = 4.01
[11:39] Stirrer speed set to 0
[11:55] Datapoint id 9 collected
[11:55] Charge balance equation is out by -26.9%
[11:55] Stirrer speed set to 50
[12:00] pH 4.22 -> 4.42

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[12:00] Using cautious pH adjust
[12:00] Dispensed 0.000776 mL of Base (0.5 M KOH)
[12:05] Stepping pH = 4.49
[12:20] Stirrer speed set to 0
[12:45] Datapoint id 10 collected
[12:45] Charge balance equation is out by 50.0%
[12:45] Stirrer speed set to 50
[12:50] pH 5.50 -> 5.70
[12:50] Using cautious pH adjust
[12:50] Dispensed 0.000118 mL of Base (0.5 M KOH)
[12:55] Stepping pH = 5.66
[12:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:00] Stepping pH = 5.88
[13:16] Stirrer speed set to 0
[13:43] Datapoint id 11 collected
[13:43] Charge balance equation is out by 40.8%
[13:43] Stirrer speed set to 50
[13:48] pH 6.03 -> 6.23
[13:48] Using cautious pH adjust
[13:48] Dispensed 0.000047 mL of Base (0.5 M KOH)
[13:53] Stepping pH = 6.09
[13:53] Dispensed 0.000071 mL of Base (0.5 M KOH)
[13:59] Stepping pH = 6.65
[14:14] Stirrer speed set to 0
[15:14] Datapoint id 12 collected
[15:14] Charge balance equation is out by -9.8%
[15:14] Stirrer speed set to 50
[15:19] pH 7.55 -> 7.75
[15:19] Using charge balance adjust
[15:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[15:39] Stirrer speed set to 0
[16:38] Datapoint id 13 collected
[16:38] Charge balance equation is out by -97.4%
[16:38] Stirrer speed set to 50
[16:43] pH 7.40 -> 7.60
[16:43] Using cautious pH adjust
[16:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[16:48] Stepping pH = 7.41
[16:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[16:53] Stepping pH = 7.62
[17:08] Stirrer speed set to 0
[18:08] Datapoint id 14 collected
[18:08] Charge balance equation is out by -248.2%
[18:08] Stirrer speed set to 50
[18:13] pH 7.67 -> 7.87
[18:13] Using cautious pH adjust
[18:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[18:18] Stepping pH = 7.62
[18:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[18:23] Stepping pH = 7.86
[18:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[18:29] Stepping pH = 8.40
[18:44] Stirrer speed set to 0
[19:37] Datapoint id 15 collected
[19:37] Charge balance equation is out by -741.2%
[19:37] Stirrer speed set to 50
[19:42] pH 8.40 -> 8.60
[19:42] Using cautious pH adjust
[19:42] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[19:47] Stepping pH = 8.38
[19:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[19:53] Stepping pH = 8.35
[19:53] Dispensed 0.000188 mL of Base (0.5 M KOH)
[19:58] Stepping pH = 9.41
[20:13] Stirrer speed set to 0
[20:30] Datapoint id 16 collected
[20:30] Charge balance equation is out by -1,840.2%
[20:30] Titration 2 of 3
[20:30] Adding initial titrants
[20:30] Automatically add 0.02500 mL of Octanol
[20:31] Dispensed 0.025000 mL of Octanol
[20:31] Stirrer speed set to 10
[20:32] Stirrer speed set to 55
[20:32] Iterative adjust 9.57 -> 2.00
[20:32] pH 9.57 -> 2.00
[20:33] Dispensed 0.057596 mL of Acid (0.5 M HCl)
[21:23] Stirrer speed set to 0
[21:33] Datapoint id 17 collected
[21:33] Stirrer speed set to 55
[21:39] pH 1.96 -> 2.16
[21:39] Using cautious pH adjust
[21:39] Dispensed 0.009454 mL of Base (0.5 M KOH)
[21:44] Stepping pH = 2.04
[21:44] Dispensed 0.007502 mL of Base (0.5 M KOH)
[21:49] Stepping pH = 2.12
[21:50] Dispensed 0.002352 mL of Base (0.5 M KOH)
[21:55] Stepping pH = 2.16
[22:10] Stirrer speed set to 0
[22:20] Datapoint id 18 collected
[22:20] Charge balance equation is out by -2.0%
[22:20] Stirrer speed set to 55
[22:25] pH 2.19 -> 2.39
[22:25] Using charge balance adjust
[22:25] Dispensed 0.011218 mL of Base (0.5 M KOH)
[22:45] Stirrer speed set to 0
[22:55] Datapoint id 19 collected
[22:55] Charge balance equation is out by 1.0%
[22:55] Stirrer speed set to 55
[23:01] pH 2.40 -> 2.60
[23:01] Using charge balance adjust
[23:01] Dispensed 0.006961 mL of Base (0.5 M KOH)
[23:21] Stirrer speed set to 0
[23:31] Datapoint id 20 collected
[23:31] Charge balance equation is out by -20.4%
[23:31] Stirrer speed set to 55
[23:36] pH 2.57 -> 2.77
[23:36] Using cautious pH adjust
[23:36] Dispensed 0.002422 mL of Base (0.5 M KOH)
[23:41] Stepping pH = 2.62
[23:42] Dispensed 0.003316 mL of Base (0.5 M KOH)
[23:47] Stepping pH = 2.73
[23:47] Dispensed 0.000917 mL of Base (0.5 M KOH)
[23:52] Stepping pH = 2.76
[24:07] Stirrer speed set to 0
[24:18] Datapoint id 21 collected
[24:18] Charge balance equation is out by -37.8%
[24:18] Stirrer speed set to 55
[24:23] pH 2.79 -> 2.99

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[24:23] Using cautious pH adjust
[24:23] Dispensed 0.001552 mL of Base (0.5 M KOH)
[24:28] Stepping pH = 2.84
[24:28] Dispensed 0.002187 mL of Base (0.5 M KOH)
[24:33] Stepping pH = 2.98
[24:33] Dispensed 0.000141 mL of Base (0.5 M KOH)
[24:38] Stepping pH = 3.00
[24:53] Stirrer speed set to 0
[25:03] Datapoint id 22 collected
[25:03] Charge balance equation is out by -25.1%
[25:03] Stirrer speed set to 55
[25:09] pH 3.03 -> 3.23
[25:09] Using cautious pH adjust
[25:09] Dispensed 0.001082 mL of Base (0.5 M KOH)
[25:14] Stepping pH = 3.07
[25:14] Dispensed 0.001952 mL of Base (0.5 M KOH)
[25:19] Stepping pH = 3.20
[25:19] Dispensed 0.000306 mL of Base (0.5 M KOH)
[25:24] Stepping pH = 3.25
[25:39] Stirrer speed set to 0
[25:50] Datapoint id 23 collected
[25:50] Charge balance equation is out by -53.6%
[25:50] Stirrer speed set to 55
[25:55] pH 3.29 -> 3.49
[25:55] Using cautious pH adjust
[25:55] Dispensed 0.000894 mL of Base (0.5 M KOH)
[26:00] Stepping pH = 3.33
[26:00] Dispensed 0.001576 mL of Base (0.5 M KOH)
[26:05] Stepping pH = 3.51
[26:20] Stirrer speed set to 0
[26:31] Datapoint id 24 collected
[26:31] Charge balance equation is out by -39.1%
[26:31] Stirrer speed set to 55
[26:36] pH 3.61 -> 3.81
[26:36] Using cautious pH adjust
[26:36] Dispensed 0.000847 mL of Base (0.5 M KOH)
[26:41] Stepping pH = 3.69
[26:41] Dispensed 0.000800 mL of Base (0.5 M KOH)
[26:46] Stepping pH = 3.90
[27:02] Stirrer speed set to 0
[27:13] Datapoint id 25 collected
[27:13] Charge balance equation is out by 2.9%
[27:13] Stirrer speed set to 55
[27:18] pH 4.16 -> 4.36
[27:18] Using charge balance adjust
[27:18] Dispensed 0.001505 mL of Base (0.5 M KOH)
[27:38] Stirrer speed set to 0
[28:00] Datapoint id 26 collected
[28:00] Charge balance equation is out by 2,543.0%
[28:00] Titration 3 of 3
[28:00] Adding initial titrants
[28:00] Automatically add 0.10000 mL of Octanol
[28:03] Dispensed 0.100000 mL of Octanol
[28:03] Stirrer speed set to 10
[28:04] Stirrer speed set to 60
[28:04] Iterative adjust 9.54 -> 2.00
[28:04] pH 9.54 -> 2.00
[28:05] Dispensed 0.060724 mL of Acid (0.5 M HCl)
[28:55] Stirrer speed set to 0

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01011**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Experiment Log (continued)

[29:06] Datapoint id 27 collected
 [29:06] Stirrer speed set to 60
 [29:11] pH 1.96 -> 2.16
 [29:11] Using cautious pH adjust
 [29:11] Dispensed 0.010042 mL of Base (0.5 M KOH)
 [29:16] Stepping pH = 2.04
 [29:16] Dispensed 0.008937 mL of Base (0.5 M KOH)
 [29:22] Stepping pH = 2.13
 [29:22] Dispensed 0.002258 mL of Base (0.5 M KOH)
 [29:27] Stepping pH = 2.16
 [29:42] Stirrer speed set to 0
 [29:52] Datapoint id 28 collected
 [29:52] Charge balance equation is out by -5.7%
 [29:52] Stirrer speed set to 60
 [29:57] pH 2.18 -> 2.38
 [29:57] Using charge balance adjust
 [29:57] Dispensed 0.012183 mL of Base (0.5 M KOH)
 [30:18] Stirrer speed set to 0
 [30:28] Datapoint id 29 collected
 [30:28] Charge balance equation is out by -10.3%
 [30:28] Stirrer speed set to 60
 [30:33] pH 2.37 -> 2.57
 [30:33] Using charge balance adjust
 [30:33] Dispensed 0.008043 mL of Base (0.5 M KOH)
 [30:53] Stirrer speed set to 0
 [31:03] Datapoint id 30 collected
 [31:03] Charge balance equation is out by -16.1%
 [31:03] Stirrer speed set to 60
 [31:08] pH 2.54 -> 2.74
 [31:08] Using cautious pH adjust
 [31:08] Dispensed 0.002775 mL of Base (0.5 M KOH)
 [31:14] Stepping pH = 2.59
 [31:14] Dispensed 0.003716 mL of Base (0.5 M KOH)
 [31:19] Stepping pH = 2.72
 [31:19] Dispensed 0.000376 mL of Base (0.5 M KOH)
 [31:24] Stepping pH = 2.75
 [31:39] Stirrer speed set to 0
 [31:49] Datapoint id 31 collected
 [31:49] Charge balance equation is out by -24.3%
 [31:49] Stirrer speed set to 60
 [31:54] pH 2.77 -> 2.97
 [31:54] Using cautious pH adjust
 [31:54] Dispensed 0.001787 mL of Base (0.5 M KOH)
 [31:59] Stepping pH = 2.82
 [32:00] Dispensed 0.002563 mL of Base (0.5 M KOH)
 [32:05] Stepping pH = 2.94
 [32:05] Dispensed 0.000423 mL of Base (0.5 M KOH)
 [32:10] Stepping pH = 2.98
 [32:25] Stirrer speed set to 0
 [32:35] Datapoint id 32 collected
 [32:35] Charge balance equation is out by -33.2%
 [32:35] Stirrer speed set to 60
 [32:40] pH 3.01 -> 3.21
 [32:40] Using cautious pH adjust
 [32:40] Dispensed 0.001246 mL of Base (0.5 M KOH)
 [32:45] Stepping pH = 3.06
 [32:46] Dispensed 0.001717 mL of Base (0.5 M KOH)
 [32:51] Stepping pH = 3.23
 [33:06] Stirrer speed set to 0

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[33:16] Datapoint id 33 collected
[33:16] Charge balance equation is out by -18.3%
[33:16] Stirrer speed set to 60
[33:21] pH 3.31 -> 3.51
[33:21] Using cautious pH adjust
[33:22] Dispensed 0.001011 mL of Base (0.5 M KOH)
[33:27] Stepping pH = 3.38
[33:27] Dispensed 0.001011 mL of Base (0.5 M KOH)
[33:32] Stepping pH = 3.56
[33:47] Stirrer speed set to 0
[33:57] Datapoint id 34 collected
[33:57] Charge balance equation is out by 0.3%
[33:57] Stirrer speed set to 60
[34:02] pH 3.70 -> 3.90
[34:02] Using charge balance adjust
[34:02] Dispensed 0.001834 mL of Base (0.5 M KOH)
[34:22] Stirrer speed set to 0
[34:52] Datapoint id 35 collected
[34:52] Charge balance equation is out by 535.4%
[34:52] Stirrer speed set to 60
[34:57] pH 6.04 -> 6.24
[34:57] Using cautious pH adjust
[34:57] Dispensed 0.000047 mL of Base (0.5 M KOH)
[35:02] Stepping pH = 6.25
[35:17] Stirrer speed set to 0
[36:17] Datapoint id 36 collected
[36:17] Charge balance equation is out by 50.0%
[36:17] Stirrer speed set to 60
[36:22] pH 6.68 -> 6.88
[36:22] Using cautious pH adjust
[36:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:27] Stepping pH = 6.69
[36:27] Dispensed 0.000047 mL of Base (0.5 M KOH)
[36:32] Stepping pH = 6.81
[36:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:37] Stepping pH = 6.99
[36:52] Stirrer speed set to 0
[37:52] Datapoint id 37 collected
[37:52] Charge balance equation is out by -157.1%
[37:52] Stirrer speed set to 60
[37:58] pH 7.09 -> 7.29
[37:58] Using cautious pH adjust
[37:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:03] Stepping pH = 7.18
[38:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:08] Stepping pH = 7.33
[38:23] Stirrer speed set to 0
[39:23] Datapoint id 38 collected
[39:23] Charge balance equation is out by -88.9%
[39:23] Stirrer speed set to 60
[39:28] pH 7.33 -> 7.53
[39:28] Using cautious pH adjust
[39:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:33] Stepping pH = 7.45
[39:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:38] Stepping pH = 7.64
[39:54] Stirrer speed set to 0
[40:54] Datapoint id 39 collected
[40:54] Charge balance equation is out by -184.4%

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 2:44:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[40:54] Stirrer speed set to 60
[40:59] pH 7.66 -> 7.86
[40:59] Using cautious pH adjust
[40:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:04] Stepping pH = 7.62
[41:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:09] Stepping pH = 7.58
[41:09] Dispensed 0.000165 mL of Base (0.5 M KOH)
[41:14] Stepping pH = 8.20
[41:29] Stirrer speed set to 0
[41:54] Datapoint id 40 collected
[41:54] Charge balance equation is out by -2,249.9%
[41:54] Stirrer speed set to 60
[41:59] pH 8.79 -> 8.99
[41:59] Using cautious pH adjust
[41:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:04] Stepping pH = 8.81
[42:04] Dispensed 0.000047 mL of Base (0.5 M KOH)
[42:09] Stepping pH = 8.88
[42:09] Dispensed 0.000047 mL of Base (0.5 M KOH)
[42:14] Stepping pH = 9.00
[42:29] Stirrer speed set to 0
[42:47] Datapoint id 41 collected
[42:47] Charge balance equation is out by -246.2%
[42:47] Stirrer speed set to 60
[42:52] pH 8.96 -> 9.05
[42:52] Using cautious pH adjust
[42:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:57] Stepping pH = 8.95
[42:57] Dispensed 0.000047 mL of Base (0.5 M KOH)
[43:02] Stepping pH = 9.06
[43:17] Stirrer speed set to 0
[43:40] Datapoint id 42 collected
[43:40] Charge balance equation is out by -272.1%
[43:40] Argon flow rate set to 0
[43:44] Titrator arm moved over Titration position